SIMULATION OF PHASE SEPARATION PHENOMENON USING LATTICE BOLTZMANN METHODS

MOHD SUHAIMI BIN TAMBONG

Report submitted in partial fulfilment of the requirements
for the award of Bachelor of Mechanical Engineering with Automotive Engineering

Faculty of Mechanical Engineering
UNIVERSITI MALAYSIA PAHANG

November 2009

SUPERVISOR'S DECLARATION

We hereby declare that we have checked this project report and in our opinion this project is satisfactory in terms of scope and quality for the award of the degree of Bachelor of Mechanical Engineering with Automotive Engineering.

Signature :
Name of Supervisor : Nik Mohd Izual bin Haji Nik Ibrahim
Position : Lecturer of Faculty of Mechanical Engineering
Date :

Signature :
Name of Panel : Azizuddin Bin Abd Aziz
Position : Lecturer of Faculty of Mechanical Engineering
Date :

STUDENTS DECLARATION

I hereby declare that the work in this report is my own expect for quotations and summaries which have been duly acknowledged. The report has not been accepted for any degree and is not concurrently submitted for award of other degree.

Signature :
Name : Mohd Suhaimi bin Tambong
ID Number : MH06060
Date :

ACKNOWLEDGEMENTS

I am grateful and would like to express my sincere gratitude to my supervisor Mr. Nik Mohd Izual bin Hj Nik Ibrahim for his brilliant ideas, invaluable guidance, continuous encouragement and constant support in making this research possible. He has always impressed me with his outstanding professional conduct, his strong conviction for science, and his belief that a Bachelor program is only a start of a life-long learning experience. I appreciate his consistent support from the first day I applied to PSM course to these concluding moments. I am truly grateful for his progressive vision about my work progressing, his tolerance of my naive mistakes, and his commitment to my future career. I also would like to express very special thanks again to my supervisor for his suggestions and co-operation throughout the study. I also sincerely thanks for the time spent proofreading and correcting my many mistakes.

My sincere thanks go to all staff of the Faculty of Mechanical Engineering, UMP, who helped me in many ways and made my stay at UMP pleasant and unforgettable. Many special thanks go to my fellow friends for their excellent cooperation, inspirations and supports during this study. I acknowledge my sincere indebtedness and gratitude to my parents for their love, dream and sacrifice throughout my life. I cannot find the appropriate words that could properly describe my appreciation for their devotion, support and faith in my ability to attain my goals. Special thanks should be given to my fellow members. I would like to acknowledge their comments and suggestions, which was crucial for the successful completion of this study.

ABSTRACT

This thesis deals with the simulation of the phase separation of two phase flow. The lattice Boltzmann methods is one of the alternative technique to solve multiphase problem such as phase separation of two-phase flow. A derivation of the Lattice Boltzmann scheme from the classical Boltzmann equation is discussed in detail. According to the problems, a single component multiphase (SCMP) LBM is used or involved in the equation in order to solve more phase of fluids. Before that, investigation on non ideal fluid is discussed using Van der Waals fluids where the critical constant of pressure, volume and temperature is solved. By doing this, it will tell the characteristic of the liquid and gas phase. From the Maxwell equal area construction, the value of macroscopic variables, density of fluids is determined which will be code in the algorithm. The source code of the phase separation generate by considering certain criteria. The result of simulation generate from the code prove the precise of the LBM. The 101x101 lattice was used and it is proven that the phase separation formed within the time increased. It is separated into two parts of colour that described the different properties of fluid phase. This project proven the LBM is the best way to simulate phase separation.

ABSTRAK

Tesis ini adalah bertujuan untuk mengkaji pengasingan fasa bagi aliran dua fasa menggunakan kaedah LBM. LBM ini mempunyai banyak kelebihan berbanding kaedah tradisional. Dalam proses kajian ini, banyak perkara perlu diambil kira bagi mendapat keputusan yang tepat dan jitu. Objektif utama adalah pemprograman data didalam perisian FORTRAN. Dalam proses pemprograman ini, banyak persamaan telah digunakan bagi mewujudkan satu persamaan baru berdasarkan persamaan 'lattice Boltzmann'. Daripada persamaan ini, nilai awal bagi kedudukan, warna, saiz dan masa berlakunya proses ini telah dikira. Kesemua nilai-nilai awal ini telah dimasukkan kedalam program komputer bagi menghasilkan keputusan kajian ini. Setelah diteliti dan diamati, keputusan kajian ini membuktikan bahawa pengasingan fasa akan berlaku secara perlahan pada kadar peningkatan tempoh tertentu. Cecair-cecair ini akan terasing secara sendiri berdasarkan ketupatan cecair masing-masing dan ini boleh dilihat daripada pengasingan warna daripada keputusan kajian. Daripada kajian ini, pembuktian tentang keberkesanan menggunakan LBM berbanding kaedah tradisional telah diketahui berdasarkan keputusan yang tepat dan jitu.

TABLE OF CONTENTS

		Page
SUPERVISOR'S DECLARATION		ii
STUDENT'S DECLARATION		iii
ACKNOWLEDGEMENTS		iv
ABSTRACT		v
ABSTRAK		vi
TABLE OF CONTENTS		vii
LIST OF TABLES		x
LIST OF FIGURES		xi
LIST OF SYMBOLS		xii
LIST OF ABBREVIATIONS		xiv
CHAPTER 1	**INTRODUCTION**	
1.1	Introduction	1
1.2	Computational Fluid Dynamics (CFD)	2
1.3	Lattice Boltzmann Methods (LBM)	4
1.4	Problem Statement	5
1.5	The Objectives of the Project	5
1.6	Scopes of the Project	5
CHAPTER 2	**LITERATURE REVIEW**	
2.1	Introduction	6
2.2	Classical Boltzmann Equation	7
2.3	Boltzmann Collision Operator	9
2.4	Bhatnagar Gross-Krook Collision Model	10
2.5	The Lattice Boltzmann Equation	11
2.6	Isothermal Lattice Boltzmann Models	12

2.7	Boundary Conditions	14
	2.7.1 Periodic Boundary Condition	14
	2.7.2 Free Slip Boundary Condition	15
	2.7.3 Bounce Back Boundary Condition	16
2.8	Relaxation Time	16

CHAPTER 3 MULTIPHASE

3.1	Introduction	18
3.2	Van der Waals Fluids	19
3.3	The Lattice Boltzmann Models	22
	3.3.1 Free Energy Lattice Boltzmann	22
	3.3.2 Thermodynamics of The Fluids	27

CHAPTER 4 METHODOLOGY

4.1	Introduction	31
4.2	The Flow Chart	31
4.3	Simulation Algorithm of Multiphase Flow	33

CHAPTER 5 RESULT AND DISCUSSION

5.1	Introduction	34
5.2	Result and Discussion	34
	5.2.1 Two Phase Flow LBM Model	34

CHAPTER 5 CONCLUSION AND RECOMMENDATION

6.1	Introduction	38
6.2	Conclusion	38
6.3	Recommendation	39

REFFERENCES 40

APPENDICES 43

A Gantt Chart of the Final Year Project 44

B Source Coding of Phase Separation 45

LIST OF TABLES

Table No.		Page
1.1	Compelling reason to use CFD	3
5.1	Parameter used for simulation phase separation	34

LIST OF FIGURES

Figure No.		Page
1.1	General concept of LBM	5
2.1	Discrete lattice velocity model	8
2.2	Streaming and collision of LBM	9
2.3	Periodic boundary condition	15
2.4	Free slip boundary condition	15
2.5	Bounce back boundary condition	16
2.6	Time relaxation concept	17
3.1	Isotherm plot of p-v diagram	21
3.2	Initial condition of particles	26
3.3	Translation (streaming) of the particles	26
3.4	Collision of the particles	26
4.1	The flow chart of the project	32
4.2	Algorithm of LBM for multiphase	33
5.1	Time evaluation of density distribution	35

LIST OF SYMBOL

ρ	Density
e_i	Lattice vector
c	Lattice velocity
w_i	Weighting factor
f, g	Distribution functions
Ω_i	Collision operator
k	Phase (k=β or k=α)
τ	Relaxation parameter
v	Kinematic viscosity
p	Pressure
f^{eq}	Equilibrium distribution function
u	Velocity
r_i	Coefficients for $\rho_\beta \neq \rho_\alpha$
s_i	Surface tension force (color-fluid model)
κ	Local curvature (color-fluid model)
σ	Surface tension coefficient
VOF	Volume of fluid function
δ	Fluid-separation coefficient
λ	Coefficient-two-relaxation-time collision
V_{inter}	Velocity on the outer side of the interface
n_k	Number density $n_k = \rho_k / m_k$
m_k	Initial density
u^{eq}	Modified equilibrium velocity
$F_k(x)$	Interactive force
μ	Chemical potential
P_{kl}	Pressure tensor
n	Total number density

φ	Number density difference between the two fluids
ϕ	Order parameter
ϕ^*	Expected order parameter
F_s	Surface tension force
T	Bulk temperature
R	Gas constant
μ	Dynamic viscosity
Re	Reynolds number

LIST OF ABBREVIATION

LBM	Lattice Boltzmann method
CFD	Computational Fluid Dynamics
LBE	Lattice Boltzmann Equations
BGK	Bhatnagar-Gross-Krook (collision operator)
VOF	Volume of fluid
LSM	Level set method
LGA	Lattice-gas automata
CSF	Continuum surface force
EOS	Equation of state
TRT	Two-relaxation-time
TC	Test of coherence
PA	physical test-case compared with an analytical solution

CHAPTER 1

INTRODUCTION

1.1 Introduction

Fluid dynamics is one of the science branches and it is very important in our daily lives because it touches every aspect. It will show us about the flow of the fluid and the property of the fluids in the universe. Otherwise, it is also an important knowledge for the engineering study. Power generation, automotive, aerospace and air conditioning are the example of the technology that related to the fluid dynamics.

The dynamics behavior of fluid flow can now be investigated by researchers using computers with certain software. The advances of computer programming have also helped them to do experiment repeatedly without having to install real apparatus. This has saved time and energy consumption.

Computational method has years been used to investigate the fluid flow behavior. One of the most popular methods used is the Computational Fluid Dynamics (CFD). CFD is a branch of fluid mechanics that uses numerical methods and algorithms to solve and analyze problems that involve fluid flows. Lattice Boltzmann Methods (LBM), the parts of the CFD is best used to simulate the fluid behavior.

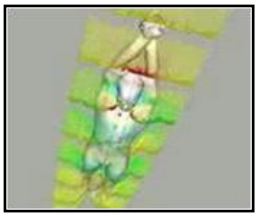
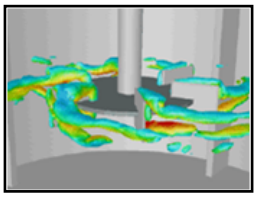
1.2 Computational Fluid Dynamics (CFD)

Computational fluid dynamics (CFD) is a computational technology that enables you to study the dynamics of things that flow. Using CFD, you can build a computational model that represents a system or device that you want to study. Then you apply the fluid flow physics and chemistry to this virtual prototype, and the software will output a prediction of the fluid dynamics and related physical phenomena.

Therefore, CFD is a sophisticated computationally-based design and analysis technique. CFD software gives you the power to simulate flows of gases and liquids, heat and mass transfer, moving bodies, multiphase physics, chemical reaction, fluid-structure interaction and acoustics through computer modeling. Using CFD software, you can build a 'virtual prototype' of the system or device that you wish to analyze and then apply real-world physics and chemistry to the model, and the software will provide you with images and data, which predict the performance of that design.

The fundamental basis of almost all CFD problems is the Navier-Stokes equations, which define any single-phase fluid flow. These equations can be simplified by removing terms describing viscosity to yield the Euler equations. Further simplification, by removing terms describing vorticity yields the full potential equations. Finally, these equations can be linearized to yield the linearized potential equations. There are three compelling reasons to use CFD software: insight, foresight, and efficiency.

Table 1.1: Compelling reason to used CFD

Insight 	CFD analysis is able to virtually crawl inside the design and see how it performs. There are many phenomenons that can witness through CFD, which wouldn't be visible through any other means, gives a deeper insight into the designs [15].
Foresight 	Because CFD is a tool for predicting what will happen under a given set of circumstances, it can quickly answer many' questions. This CFD will give the outcomes or results of the numerical set of boundary conditions. All of this can be done before physical prototyping and testing [15].
Efficiency 	The foresight that is gain from CFD helps engineer to design better and faster, save money, meet environmental regulations and ensure industry compliance. CFD analysis leads to shorter design cycles and the products get to market faster. In addition, equipment improvements are built and installed with minimal downtime. CFD is a tool for compressing the design and development cycle allowing for rapid prototyping [15].

Source: Yuan, P. et al., 2006

1.3 Lattice Boltzmann Methods (LBM)

LBM is a relatively new simulation technique for complex fluid systems and has attracted interest from researchers in computational physics. Unlike the traditional CFD methods, which solve the conservation equations of macroscopic properties (i.e., mass, momentum, and energy) numerically, LBM models the fluid consisting of fictive particles, and such particles perform consecutive propagation and collision processes over a discrete lattice mesh. Figure 1.1 shows the explanation of the basic concept of the LBM. Due to its particulate nature and local dynamics, LBM has several advantages over other conventional CFD methods, especially in dealing with complex boundaries, incorporating of microscopic interactions, and parallelization of the algorithm. A different interpretation of the lattice Boltzmann equation is that of a discrete-velocity Boltzmann equation. The numerical methods of solution of the system of partial differential equations then gives rise to a discrete map, which can be interpreted as the propagation and collision of fictitious particles [1] [2].

Simulating multiphase flows has always been a challenge to conventional CFD because of the moving and deformable interfaces. More fundamentally, the interfaces between different phases (liquid and vapor) or components (e.g., oil and water) originate from the specific interactions among fluid molecules. Therefore it is difficult to implement such microscopic interactions into the macroscopic Navier–Stokes equation. However, in LBM, the particulate kinetics provides a relatively easy and consistent way to incorporate the underlying microscopic interactions by modifying the collision operator. Several LBM multiphase models have been developed [3]. Phase separations are generated automatically from the particle dynamics and no special treatment is needed to manipulate the interfaces as in traditional CFD methods. Successful applications of multiphase LBM models can be found in various complex fluid systems, including interface instability, bubble/droplet dynamics, wetting on solid surfaces, interfacial slip, and droplet electro hydrodynamic deformations.

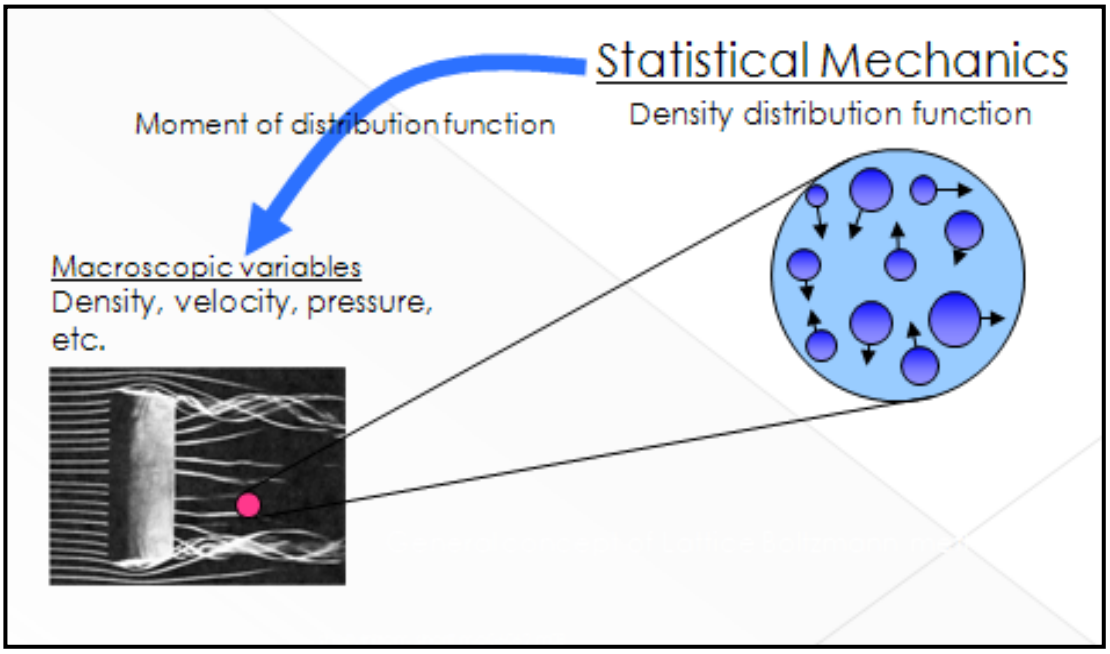


Figure 1.1: General concept of LBM

Source: Nik Mohd Izual, 2009

1.4 Problem Statement

The problem statement regarding this project is stated below:

- Most complex fluid dynamics problems cannot be solved analytically but can be analyze by using code of LBM.

1.5 Objective

The objective of this project is to simulate phase separation phenomenon using Lattice Boltzmann Methods (LBM).

1.6 Scopes

1. Literature review of lattice Boltzmann method (LBM).
2. Use free energy (FE) parameters proposed by Nik Mohd Izual [28].
3. Simulate the phase separation of LBM.

CHAPTER 2

LITERATURE REVIEW

2.1 Introduction

Lattice Gas Cellular Automata (LGCA) and Lattice Boltzmann Method (LBM) are relatively new and promising methods for the solution of nonlinear partial differential equations and simulation of fluid flows. In the last few years, a remarkable development has been taken place in (LBM) [1-6]. Lattice Boltzmann models have ability to simulate single and multi-phase flows of single and multicomponent fluids. Historically the LBM evolves from LGCA which belongs to the class of cellular automata that are used for simulation of the fluid flow phenomena. It represents an idealization of the physical system in which space and time both are discrete. In 1986, Frisch, Hasslacher, and Pomeau and Wolfram proposed the first two-dimensional lattice gas automaton model for the specific purpose of computational fluid dynamics [7].

In 1988, a proposal to use the lattice Boltzmann equation to simulate fluid flow problems was made for the first time [6]. The kinetic nature of LBM has several distinct features different from other computational fluid dynamics (CFD) approaches that are used to solve the Navier Stokes equations. The convection operator in LBM is linear in phase space, similar to that of the Boltzmann kinetic equation, but different than the Euler or the Navier Stokes equations and pressure is obtained through an equation of state, instead of solving a Poisson equation as in the incompressible Navier Stokes equations. LBM uses minimum set of discrete velocities so that the conserved quantities remain preserved throughout the simulation.

Researchers have used LGCA and LBM for a variety of fluid flow problems and geometries. A rich variety of behaviors including unsteady flows, phase separation, evaporation, condensation, cavitations, porous media flows, blood flow simulation, solute and heat transport, buoyancy, multiphase flows, compressible flows and interactions with surfaces can readily be simulated [8-25]. Various fluid flow problems have been simulated using LGCA and results have been compared with experimental investigations [8]. LGCA has been used to investigate flow through geometrically irregular media [11].

An LGCA model with non-ideal equation of state has been presented to simulate the transition from solid to gas phase [12]. LBM has been used to numerically analyze the turbulent shear flows [13]. Results obtained for three-dimensional low Reynolds number flows, using LBM, demonstrate the viability of the method for such flows in complex geometries [14]. LBM is equally applicable for simulation of multiphase flows. LB Models have been formulated for two-dimensional multiphase flows in porous media [15]. Many researchers have formed thermal models to investigate heat conduction process and convective flows by using LBM [20, 23]. LBM has even been used to simulate shock wave phenomena [25].

2.2 Classical Boltzmann Equation

LBM is relatively recent technique that has been shown to be as accurate as traditional CFD methods having the ability to integrate arbitrarily complex geometries at a reduced computational cost. Lattice Boltzmann models vastly simplify Boltzmann's original conceptual view by reducing the number of possible particle spatial positions and microscopic momenta from a continuum to just a handful and similarly discretizing time into discrete steps. Figure 2.1 shows that particle positions are confined to the node of a lattice. Variations in momenta that could have been due to a continuum of velocity directions and magnitudes and varying particle mass are reduced to eight directions leading to a D2Q9 model.

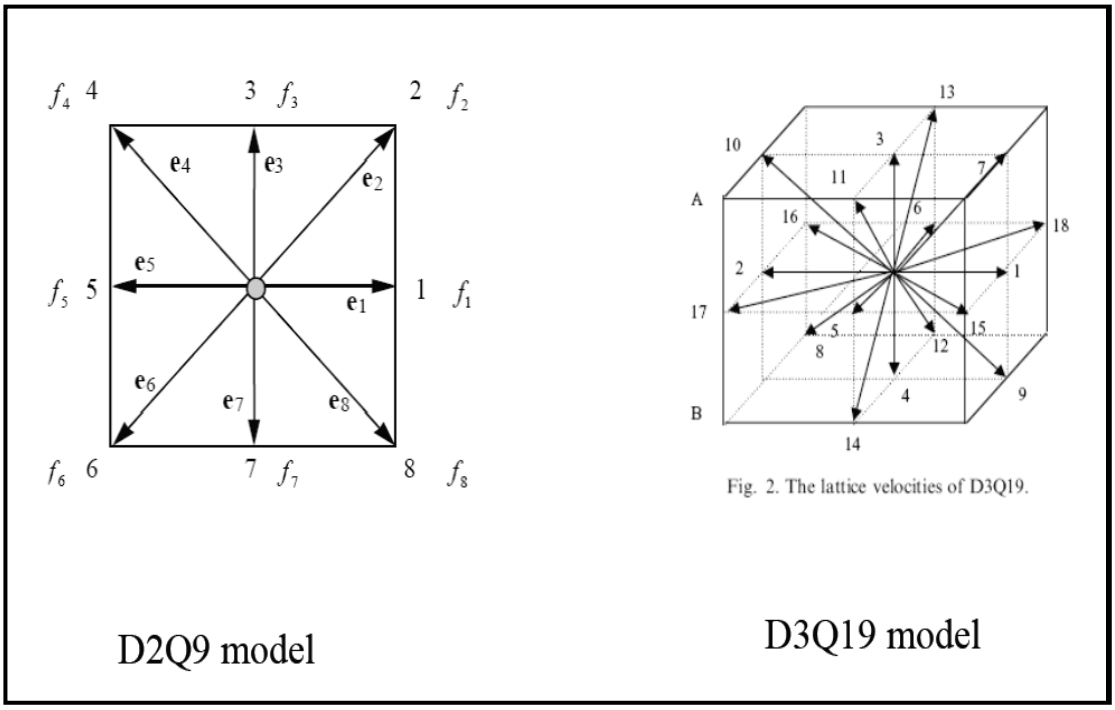


Fig. 2. The lattice velocities of D3Q19.

Figure 2.1: Discrete lattice velocity model

Source: Grunau, D., et al., 1993

Lattice Boltzmann equation can be obtained directly from the lattice gas automata by taking ensemble average with the assumption of random phase, leading to the following equation [26];

$$f(x + c\Delta t, c + a\Delta t, t + \Delta t) - f(x, c, t) = \Omega_\alpha(f) \qquad (2.1)$$

Where $\Omega_\alpha(f)$ is the Lattice Boltzmann collision operator and $f(x, c, t)$ is the single particle distribution functions with discrete velocity *c*.

There are two conditions that are related to the distribution function, without collisions and with collisions [27][28]. The distribution function of $f(x, c, t)$ describes the number of particles in the situation where it is at the position of *x*, move with velocity *c* at time *t*.

At the short duration of time Δt , each particle changing the velocity from c to $c + a\Delta t$ to move from x to $x + c\Delta t$, where a is an acceleration due to the external forces. The number of molecules for both $f(x, c, t)\, dx\, dc$ and $f(x + c\Delta t, c + a\Delta t, t + \Delta t)\, dx\, dc$ are same in the condition of distribution without collision. Therefore;

$$f(x + c\Delta t, c + a\Delta t, t + \Delta t)\, dx\, dc - f(x, c, t)\, dx\, dc = 0 \qquad (2.2)$$

In the condition where collision occurs, there will be a net different number of molecules between these two functions that can be express by;

$$f(x + c\Delta t, c + a\Delta t, t + \Delta t)\, dx\, dc - f(x, c, t)\, dx\, dc = \Omega_\alpha(f)\, dx\, dc\, dx\, dt \qquad (2.3)$$

After dividing this equation with *cdt*, *dt* tends to zero (*dt*~0), give the Boltzmann equation of *f*

$$\frac{\partial f}{\partial t} + c_\alpha \frac{\partial f}{\partial c_\alpha} + a \frac{\partial f}{\partial c_\alpha} = \Omega(f) \qquad (2.4)$$

2.3 Boltzmann Collision Operator

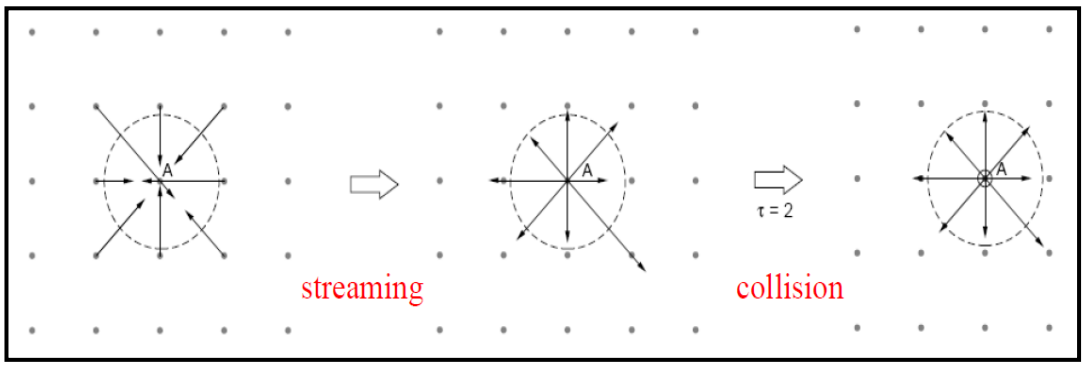


Figure 2.2: Streaming and collision of LBM

Source: Zhang, R., et al., 1999

An expression of the collision operator is required for any solution of Boltzmann equation.

$$\int \begin{bmatrix} 1 \\ c \\ c^2 \end{bmatrix} \Omega(f)\, dc \tag{2.5}$$

By the way, collision operator can change the distribution function $f(x, c, t)$ in two ways;

1. After the collision, the velocities of the particle will be different from the initial velocity and this circumstances causing the decrease in $f(x, c, t)$

2. The particles that have the velocities of others will have the velocity after collision, increasing $f(x, c, t)$

2.4 Bhatnagar-Gross-Krook Collision Model

From the previous derivation of Boltzmann equation, assuming that a gas consist of hard-sphere and undergoing the binary collision [15]. There is the derivation of Boltzmann equation without external force shows that the change in distribution functions per unit time due to collision;

$$\frac{\partial f}{\partial t} + c_\alpha \frac{\partial f}{\partial c_\alpha} = \frac{\partial f}{\partial t} = \left.\frac{\partial f}{\partial t}\right|_{collision} \tag{2.6}$$

where;

$$\left.\frac{\partial f}{\partial t}\right|_{collision} = \Omega(f) \tag{2.7}$$